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Annihilation of positrons trapped at the (100) and (111) surfaces of Si

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Abstract

We present results of theoretical studies of positron surface states and positron annihilation characteristics at the clean non reconstructed (100) and (111) surfaces of Si performed within the modified atomistic, superposition method. It is found that in the case of non reconstructed semiconductor surfaces, the positron surface state is localized mainly on the vacuum side of the topmost layer. The computed positron surface state energies E_b at the (100) and (111) surfaces of Si are −2.81 and −2.69 eV. In addition, calculations of the positron work functions with respect to the vacuum for bulk Si(100) and Si(111) yielded 2.34 and 2.23 eV, respectively demonstrating the stability of positron surface state on these surfaces. The positron surface state lifetime as well as probabilities for a positron trapped in a surface state to annihilate with relevant core-level electrons are computed for both surfaces, and compared with available experimental data.

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1. Introduction

Positron bound states at metal surfaces, both clean and adsorbate-covered, have become the subject of experimental studies using positron-annihilation-induced Auger-electron spectroscopy (PAES) [1]. In PAES experiments most of the low-energy positrons, implanted into the sample under study, diffuse back to the vacuum–solid interface and are trapped into a surface state. A certain fraction of the positrons at the surface state annihilate with neighboring core-level electrons, creating core–hole excitations which give rise to Auger-electron emission. Since PAES intensities are sensitive to the spatial distribution of the positron wave function on the surfaces of interest, the method has been already used to study the nature and location of the positron surface state at clean and adsorbate covered transition-metal surfaces [2]. Recently PAES has been applied to study positron annihilation at the (100) and (111) surfaces of Si (see the Figs. 1 and 2).

This paper presents a first-principles study of the positron surface state and positron annihilation characteristics at the clean non reconstructed (100) and (111) surfaces of Si using the modified atomistic,

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